

# Concurrent materials design

**Gareth Conduit**

Patents GB1302743.8 (2013), EP14153898.3 (2014), US 2014/177578 (2014)

Patents GB1307533.8 (2013), EP14161255.6 (2014), US 2014/223465 (2014)

Patent GB1307535.3 (2013)

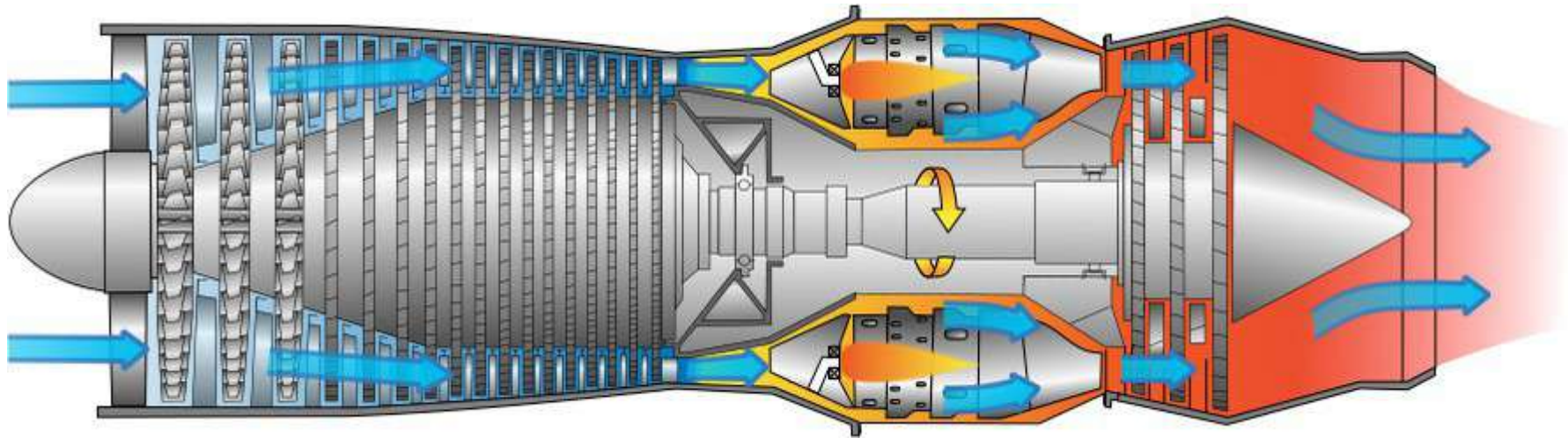
Patent US 2013/0052077 A1 (2013)

Acta Materialia, **61**, 3378 (2013)

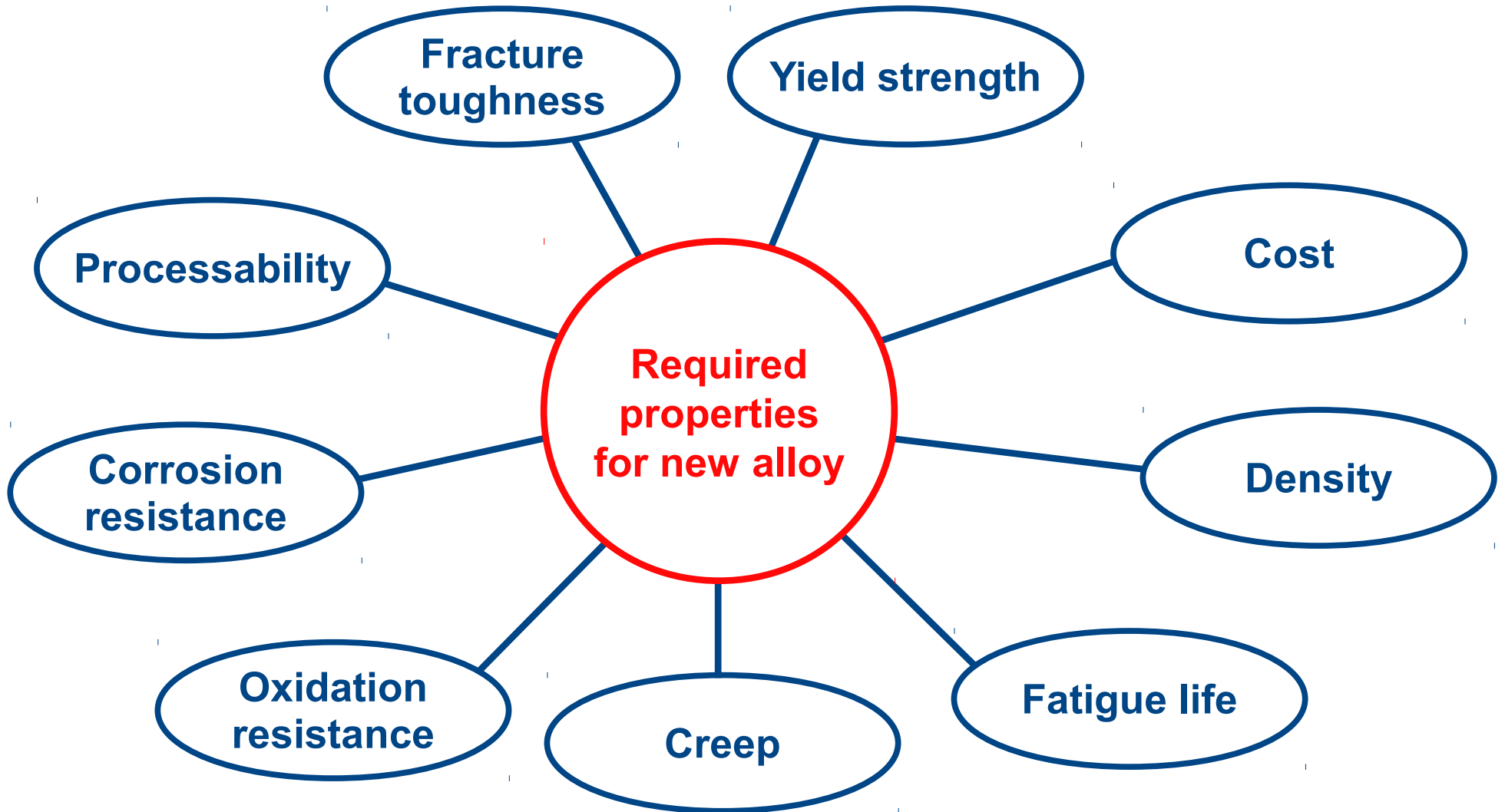
Intermetallics, **48**, 62 (2014)

**Theory of Condensed Matter Group, Department of Physics**

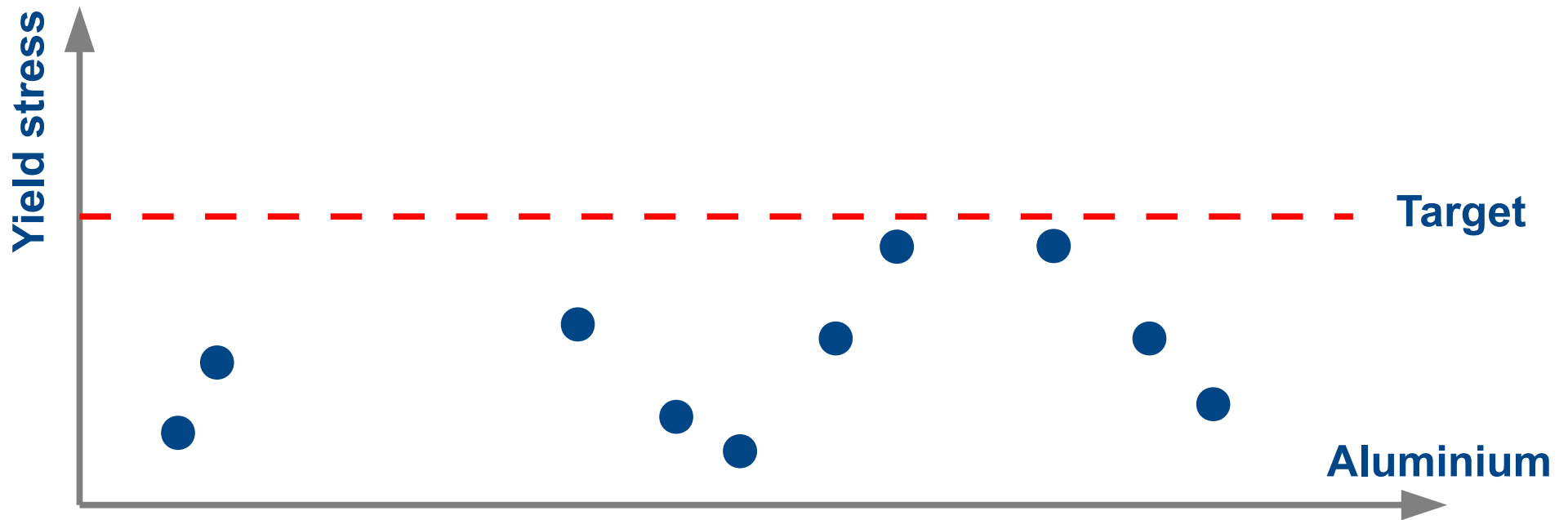
# Jet engine: turbine discs



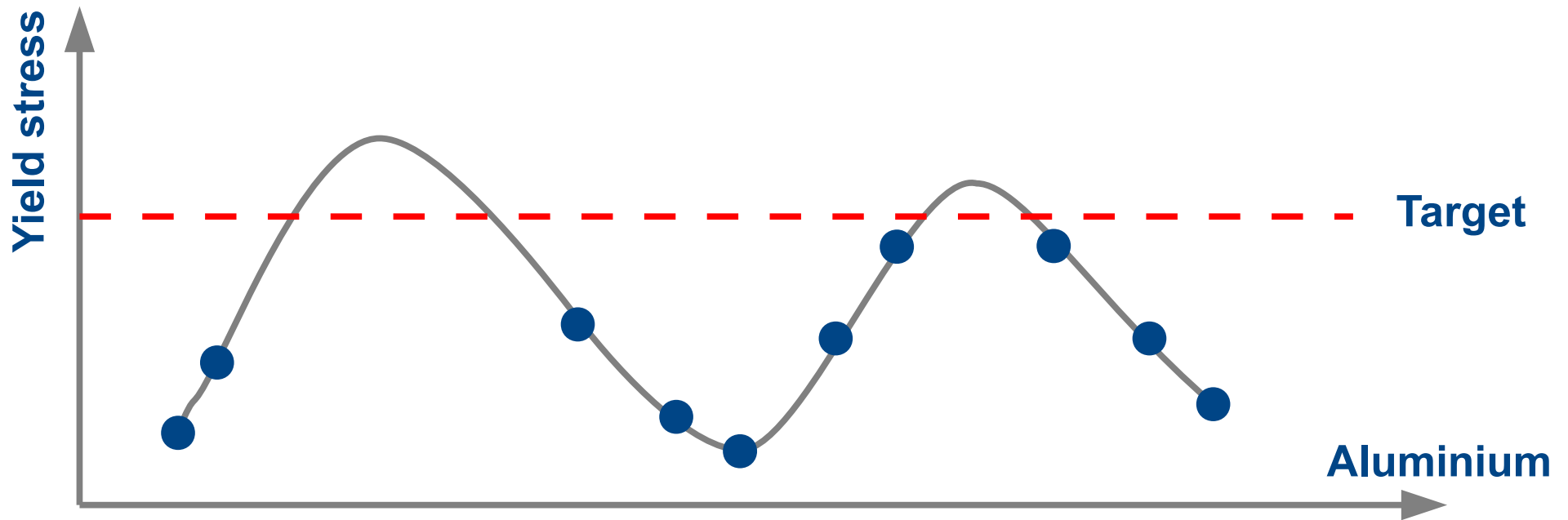
# Designing a new alloy – what is required?



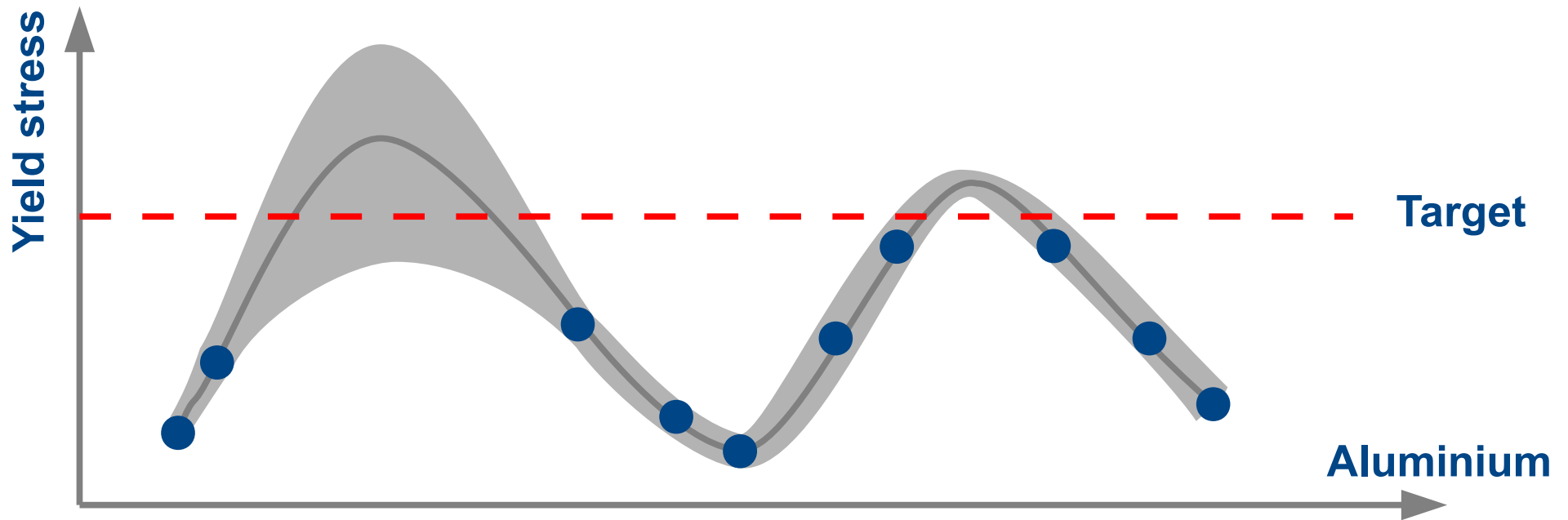
# Neural network fitting & optimization



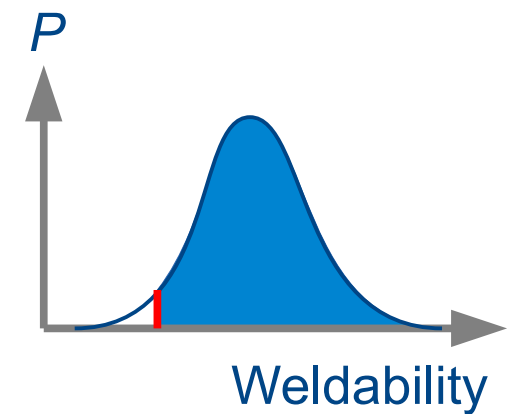
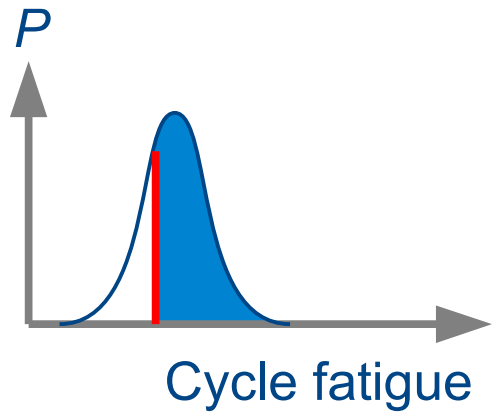
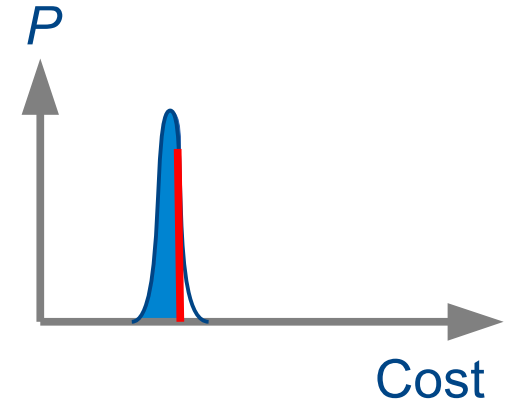
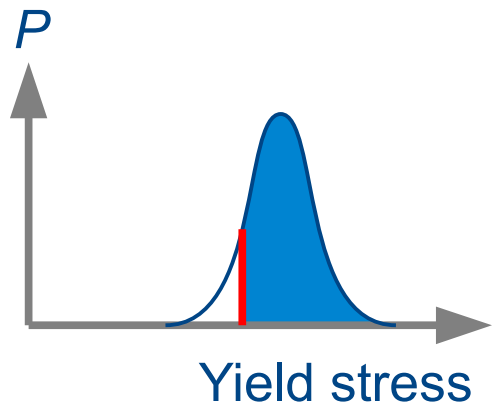
# Neural network fitting & optimization



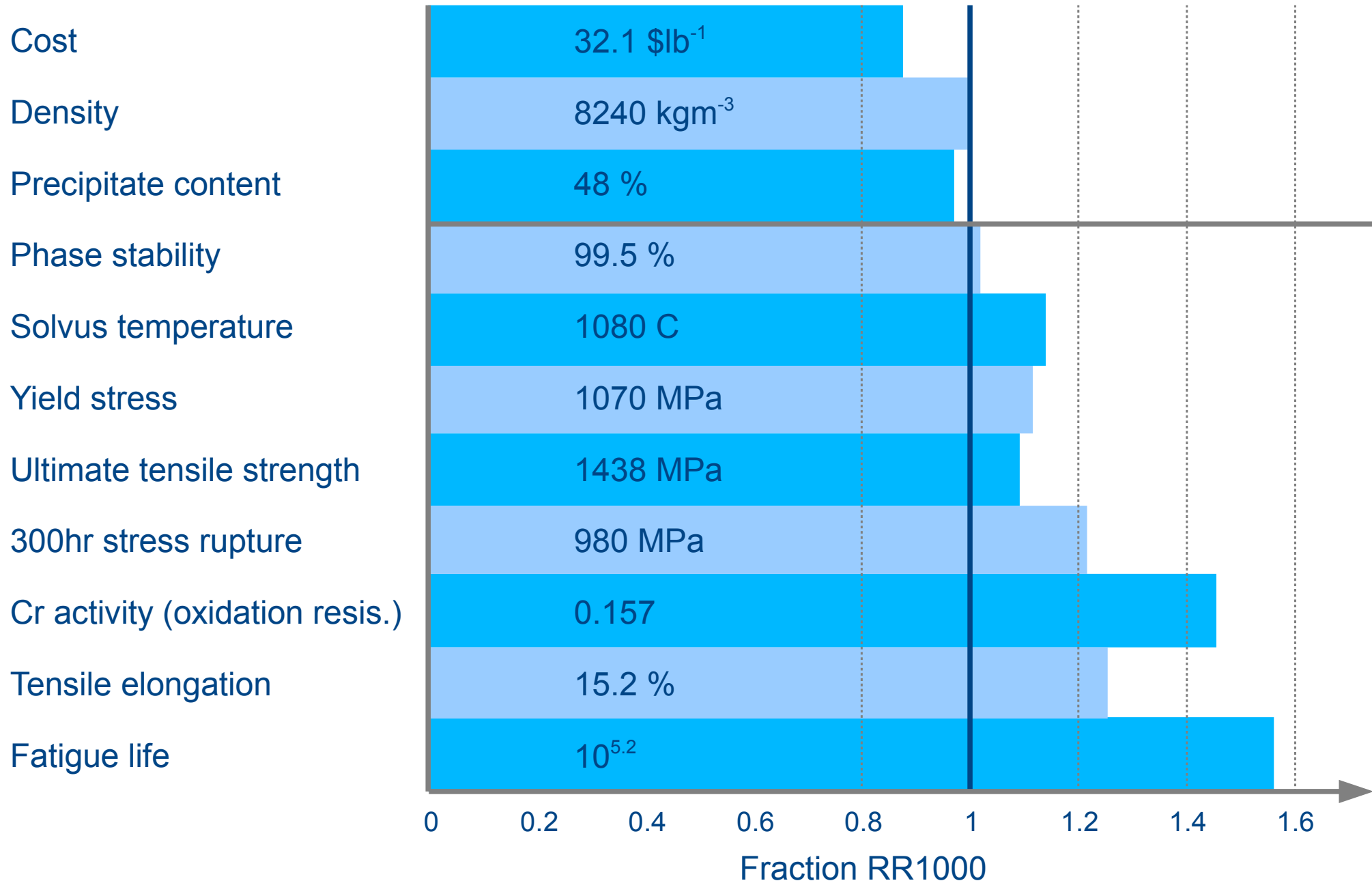
# Neural network fitting & optimization



# Probability

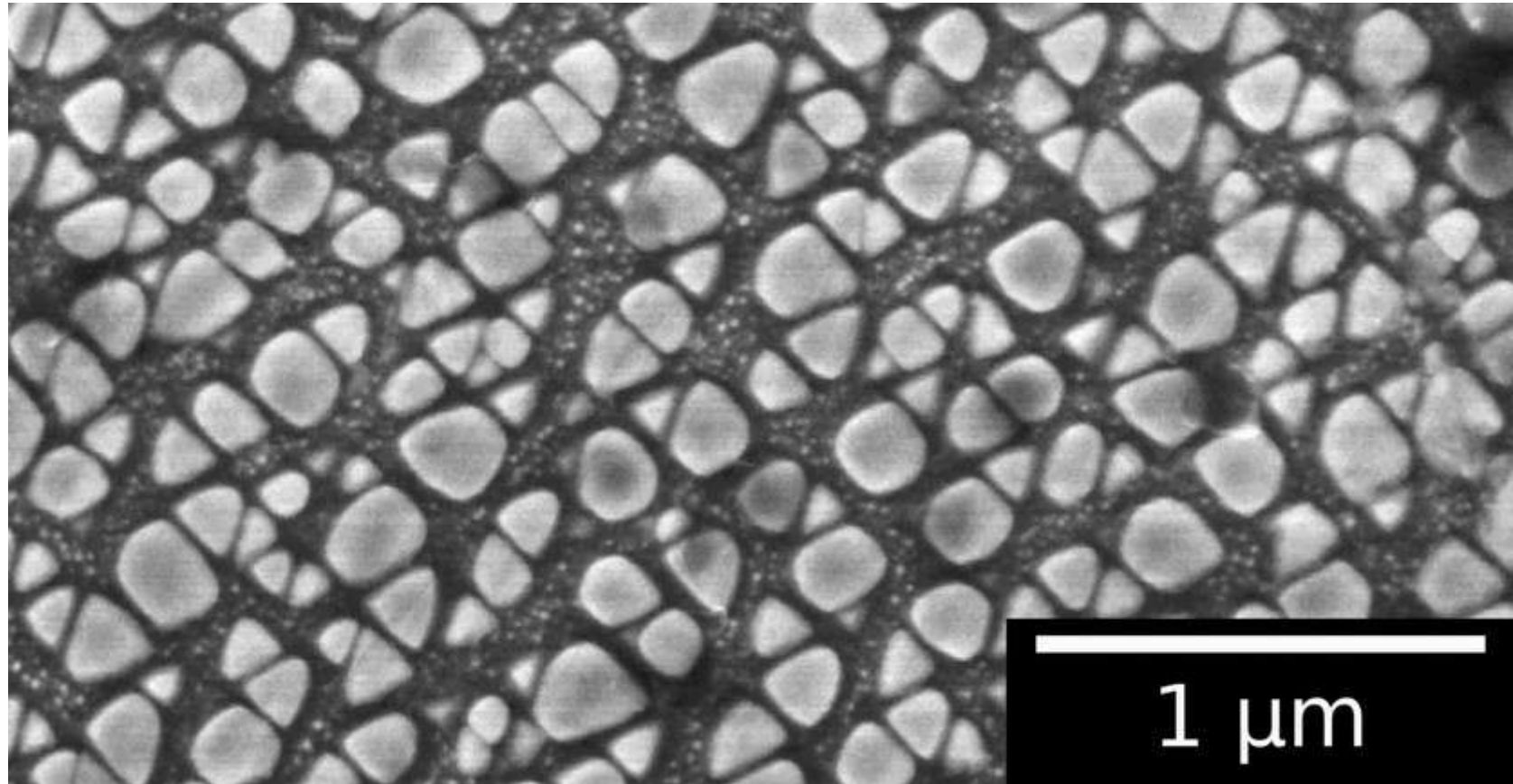


# Ni-base superalloy

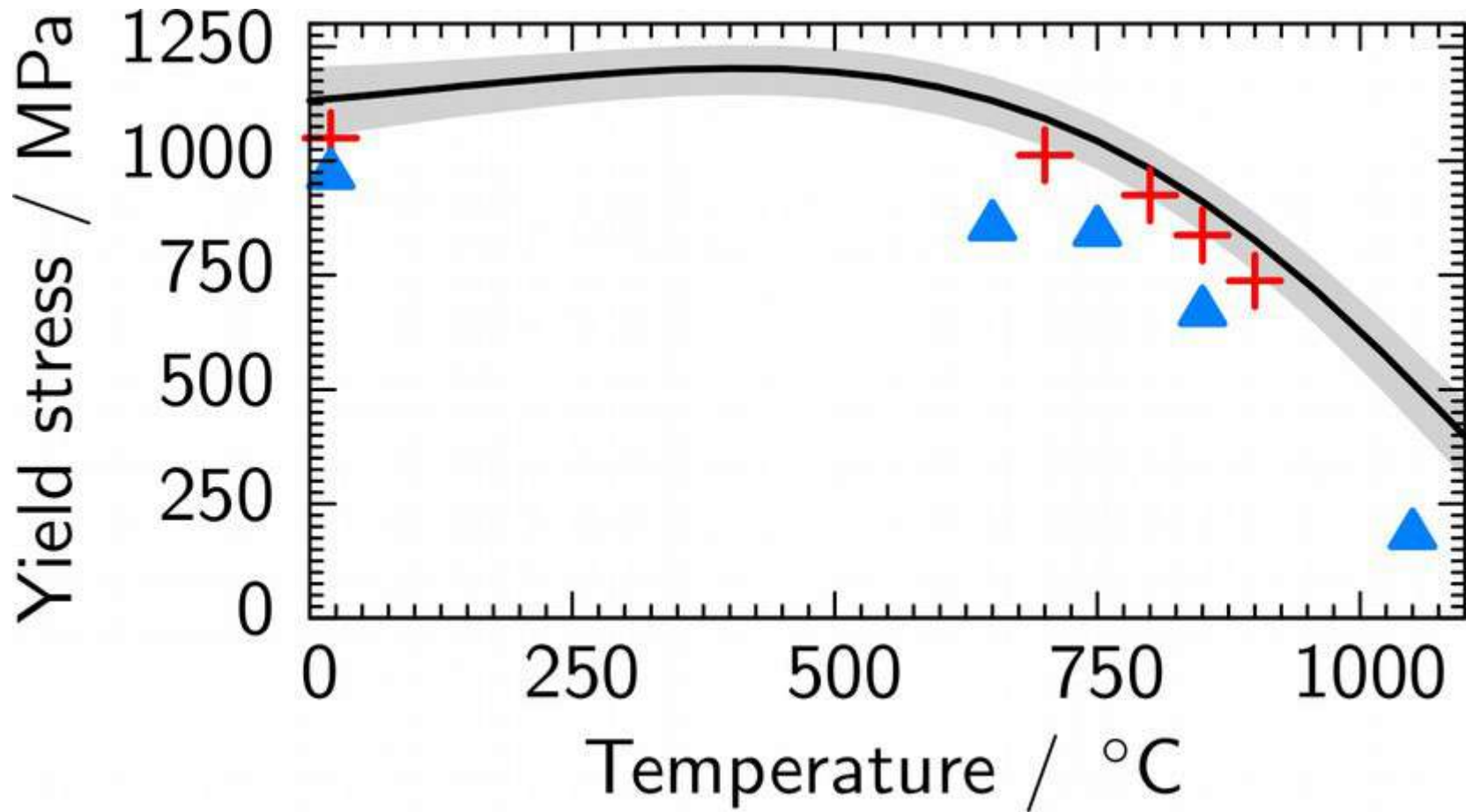




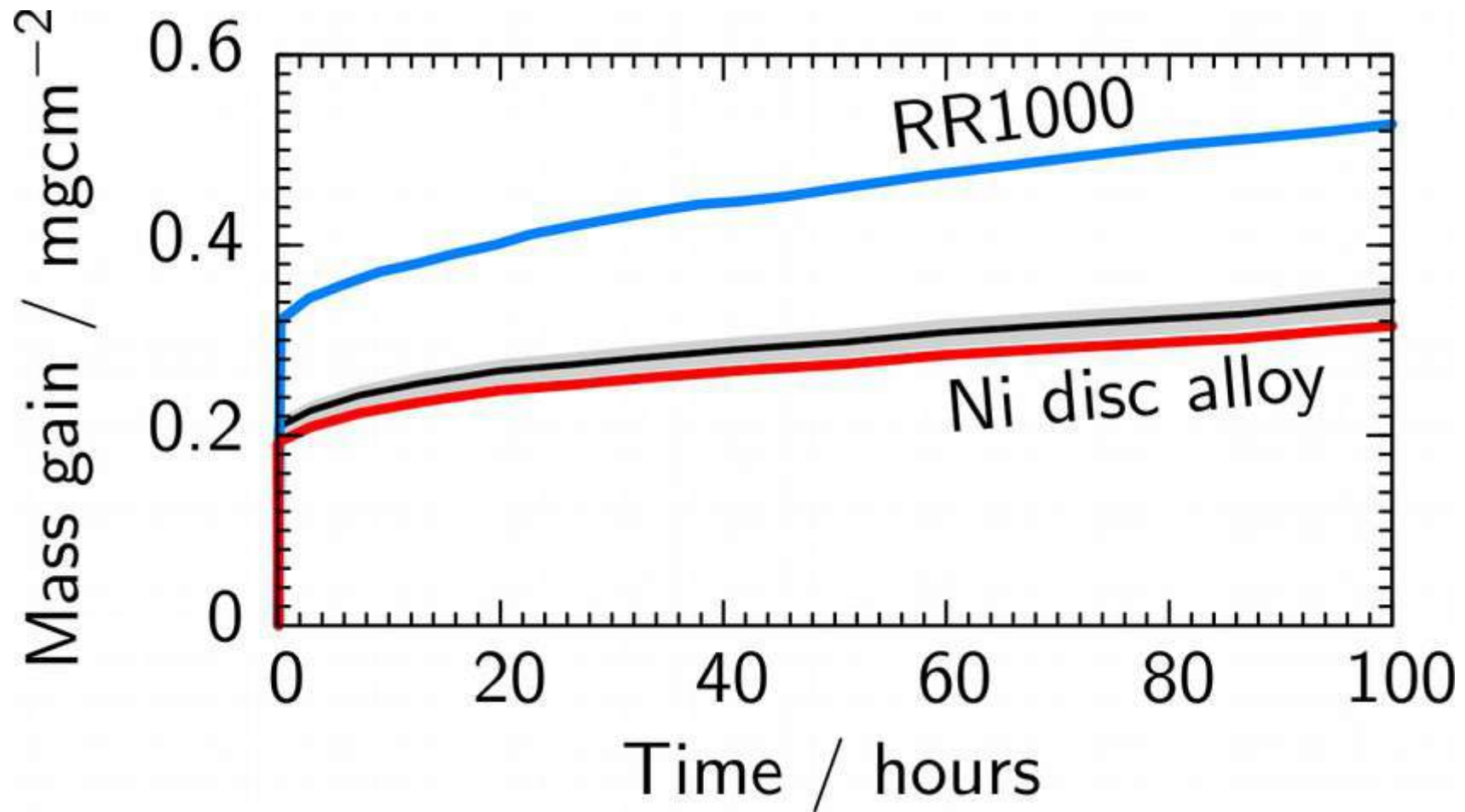
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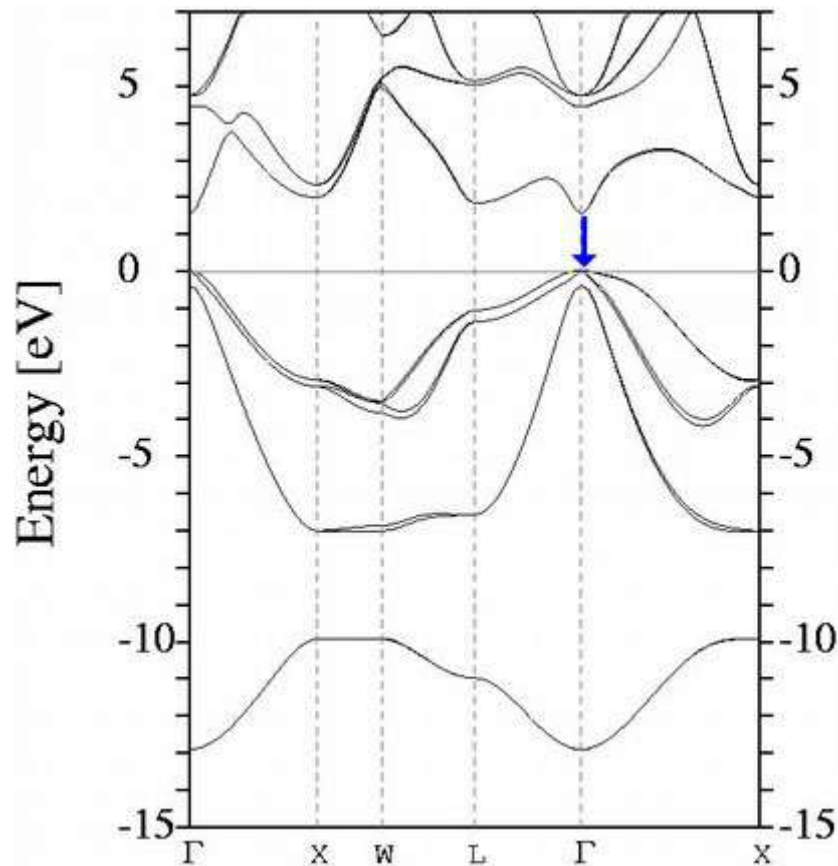
# Ni-base superalloy



# Ni-base superalloy



# Semiconductors

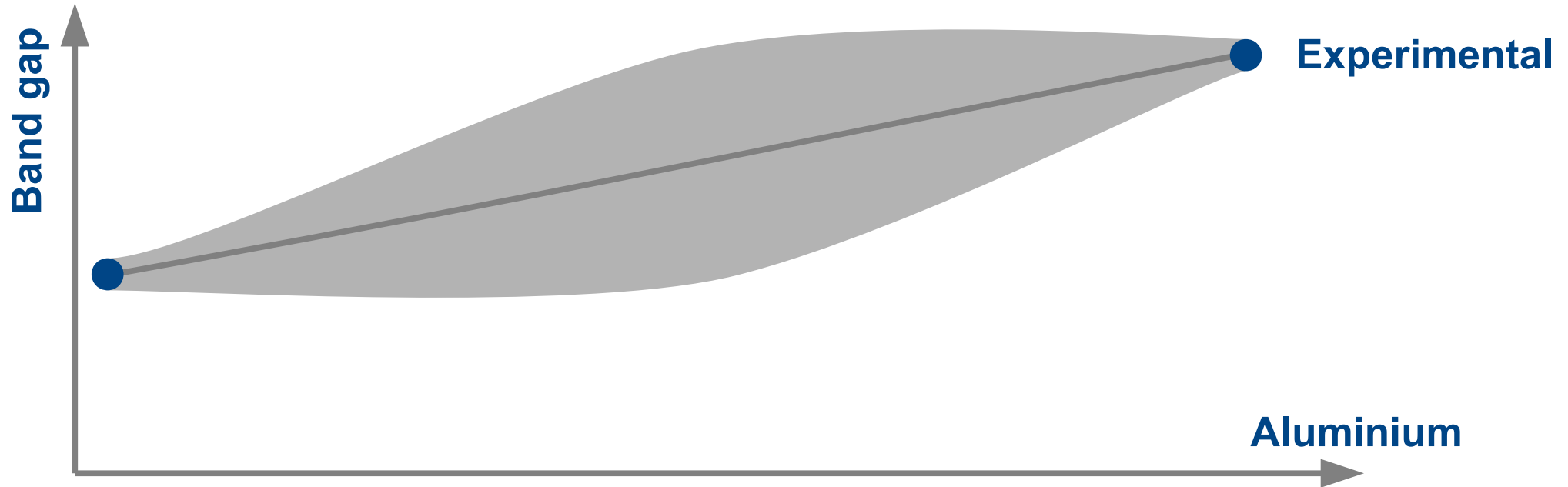


100 points for band gap, efficacy



Band structure: band gap, density of states, effective mass

# Semiconductors

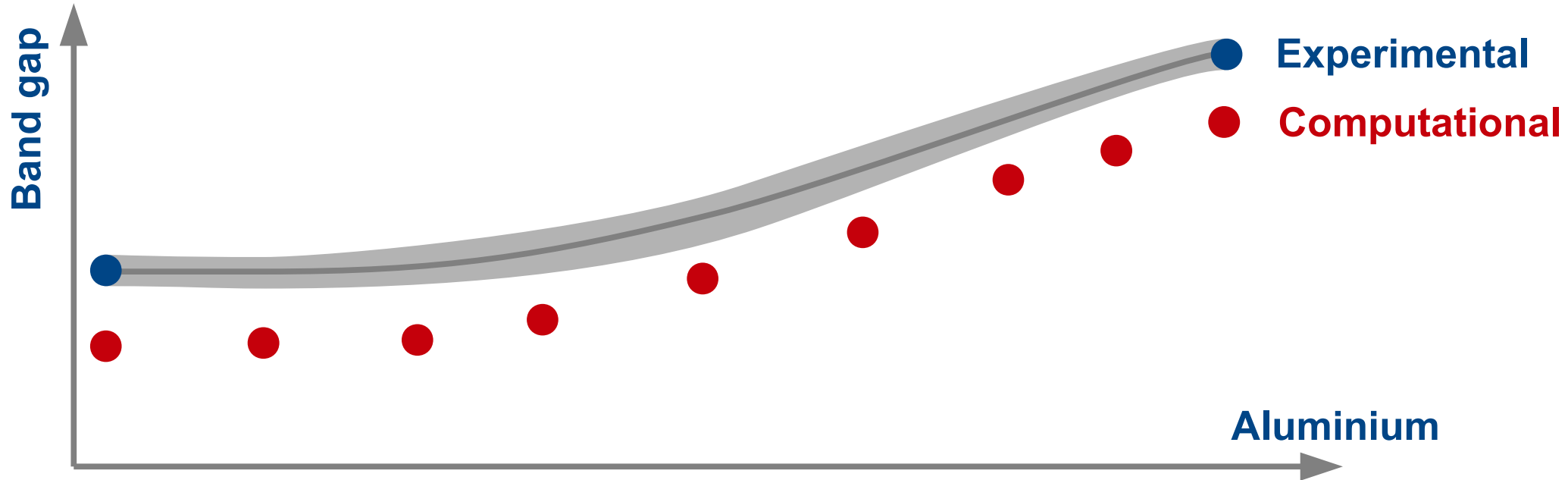


100 points for band gap, efficacy



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# Semiconductors



100 points for band gap, efficacy



Band structure: band gap, density of states, effective mass

# Prospects in the future

Take advantage of experimental databases to develop Ni and Mo-based alloys

Combine further first principles approaches to build new databases and guide extrapolation

Projects with Rolls Royce, Samsung, Royal Society Brian Mercer Feasibility award

Long-term goal of concurrent materials design